Ocean State Estimation for Climate Studies

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1. Current Status and Prospects

Climate variabilities, which are of interest to CLIVAR, involve a broad range of spatial and temporal scales. In-situ observing systems are too sparse to directly observe all important processes. Satellite measurements, although having broad sampling capabilities, are limited to surface characteristics.
Numerical ocean models are limited by uncertainties associated with surface forcing fields, model parameters, and lateral boundary conditions (for regional models). Model errors due to coarse spatial resolution and incomplete/improper representations of physical properties (e.g. dynamical and numerical truncations) provide another level of uncertainty. Therefore, ocean state estimation (often referred to as ocean data assimilation), by optimally combining observations and models, becomes an important element of CLIVAR.

A primary goal of ocean state estimation is to use observations and models to produce an estimate state of the ocean that is consistent with observations and model dynamics. When validated, the optimal solution is used to infer unobserved (or unobservable) quantities, to perform space-time interpolation/extrapolation of observable quantities, and to investigate processes associated various climate variabilities. A second goal of ocean state estimation, arguably the prerequisite of the estimation, is to test the validity of the underlying model and to identify its limitation so that improvement can be made. In addition, ocean state estimation supports the following: evaluation of the impact of a given data set in constraining the model state; the relative impacts of different data types; parameter estimation; design of observing network; improving air-sea fluxes, and determining the need of additional observations.

Typically, ocean state estimation is formulated as a least-squared problem in which a cost function of the following generic form is minimized subject to data and model dynamical constraints:

$$J = \Sigma(y(t)-H[x(t)])^{T}R^{-1}(y(t)-H[x(t)]) + \Sigma(x(t+1)-F[x(t)])^{T}Q^{-1}(x(t+1)-F[x(t)])$$

where $y(t)$ are observations distributed in space and time, $x(t)$ is the model state, H is an "observational matrix" that computes the model-equivalent of observations, $x(t+1) \approx F[x(t)]$ is the model equation that approximately describes the state evolution (the model is assumed ``perfect" if $\approx$ is replaced by $=$), and R and Q are a priori error covariance matrices for the data and model constraints, respectively. The summation is over time, reflecting the constraint on the time history of the model. The final solution is essentially a weighted least-squared fit of the model to the data. Given the data and a model, the prescription of R and Q (a priori errors of data and model constraints) dictates the outcome of the estimation.

Many methods have been devised to solve the above inverse problem. Reviews of various methods can be found in many sources (e.g., Anderson and Willebrand, 1989; Ghil and Malanotte-Rizzoli, 1991; Bennett, 1992; Wunsch, 1996; Robinson et al., 1998). The more common "advanced" methods include the adjoint (i.e., four-dimensional variational or 4D-Var), the sequential Kalman filter and related smoothers, representer, and Green's function methods. These methods differ in algorithm but are equivalent to each other so long as assumptions about data and model dynamical constraint errors (as they appear in the above expression of cost function J) are the same. Less sophisticated and computationally less expensive schemes include three-dimensional variational (3D-Var) and optimal interpolation where data and model constraints in the time dimension are not considered (i.e., missing the summation over time). There are also simple methods such as nudging and data insertion methods. Instead of formally solving for an inverse problem, these methods the model state is relaxed toward, or replaced by, by data (similar to treating model errors in J as infinite).

Data assimilation with ocean GCM using advanced methods has been demonstrated on basin to near-global scales (e.g., Yu and Malanotte-Rizzoli 1996, Lee and Marotzke 1997, Lee and Marotzke 1998, Fukumori et al.1999, Verron et al. 1999). Although being prototypes, most of these studies explicitly account for uncertainties due to surface forcing and lateral boundary conditions (for regional studies) that account for a significant portion of the model error. There are also efforts which use simpler assimilation methods but with higher-resolution models to assimilate multi-decadal hydrographic data (Ji et al. 1994, Carton et al. 2000). Assimilation of oceanic and atmospheric data into intermediate coupled ocean-atmosphere models using advanced assimilation methods has also been attempted for the tropical Pacific (e.g., Bennett et al. 1998, Lee et al. 2000, Ballabrera-Poj et al. 2001, Sun et al. 2002).

To address the ocean state estimation needs of CLIVAR and GODAE (Global Ocean Data Assimilation Experiment), a multi-institutional consortium has recently been formed under the US National Ocean partnership Program (NOPP) with funding from NSF, NASA, and ONR. The consortium is named "Estimation of the Circulation and Climate of the Ocean" (ECCO; http://www.ecco-group.org). The goal is to elevate global ocean state estimation from its current experimental status to a quasi-operational tool for climate research and to integrate the modeling and observational communities. The scientific goal is to describe and understand the global general circulation of the oceans and its role in climate by combining modern large-scale data sets with a state-of-the-art general circulation model. ECCO products are available through Live Access Data Severs (http://www.ecco-roup.org/data_server.html). The products are being used by scientists from various disciplines in studies from carbon cycle to earth rotation. An overview of the ECCO effort has been reviewed by Stammer et al. (2002).

2. Major Issues

Although the ultimate goal of ocean state estimation is clear, there are many practical issues, which hinder its progress. The following are some of the major issues.

Error prescription

The most critical aspect in ocean state estimation is determining and understanding the error covariances of data and model constraints because they dictate the outcome of the assimilation. Errors in a model solution come from many sources. Some are associated with external factors such as uncertainties in the initial state, surface fluxes, and side (open) boundary conditions or improperly prescribed values of parameters. Others are internal in nature such as inappropriate form of parameterizations (e.g. of mixing) or the errors resulting from coarse model resolution or missing physics (e.g. mesoscale eddy fluxes).

Processes not represented by the model, and thus not correctable by ocean state estimation, are referred to as model representation error (after Lorenc, 1986). This type of error is included in the data-constraint error covariance **R** to avoid forcing the model to fit parts of the data it cannot represent. As such, the data-constraint errors differ from measurement error (sampling and instrumentation errors), which is usually much smaller than the representation error. Processes resolvable by the model but incorrectly appearing in a model solution due to uncertainties of external factors (e.g., forcing), sometimes called model process noise, is included in the model-constraint error **Q**. The estimated state can then deviate from the prior model solution in such a way (as described by **Q**) to account for uncertainties in external factors. Recognizing the sources of model errors and correctly attributing them in **R** and **Q** alleviates the risk of a biased estimation.

Assimilation can correct errors from external factors by treating the initial state, surface fluxes, open boundary conditions, or mixing coefficients as control variables and solving for their optimal values. In principle, internal model errors must be corrected in the context of forward model improvement although some internal error can be compensated by assimilation. For instance, incorrect stratification due to an inappropriate form of vertical diffusion parameterization can be fixed through the assimilation of density profile data (even though the source of the error is not eliminated from the model).

While estimating model errors is challenging, determining data-constraint uncertainties is also nontrivial. For example, the uncertainty of altimetric sea level data depend on errors associated with satellite orbit, tides, atmospheric corrections and the inverted barometer effect. Efforts have been made (e.g., Fu et al. 1993) to quantify the error covariance of altimeter data based on its reasonably good spatial-temporal sampling characteristics. For in-situ data such as hydrography, the point-wise measurement error is usually smaller than that of satellite data. However, the limited samples of in-situ data are often used to infer the large-scale low-frequency state of the ocean through assimilation using non-eddy resolving models. In this context, transient signals such as eddies captured by the hydrographic casts are considered "noise" and a covariance of eddy structure is needed to develop data-constraint error covariance. These eddy statistics are difficult to estimate from the limited sampling in space and time that is now available. Knowledge of model errors depends critically on the amount of available data. Because the difficulty in estimating model errors is primarily due to the lack of sufficient samples, the increase in observational density will not only improve assimilation products through stronger data constraints, but also through better assessment of model errors.

Validation

An important aspect of ocean state estimation is complete evaluation of the quality of the assimilation product in order to identify inappropriate prescription of a priori errors or possible model weaknesses and to improve upon them. Similar to elementary linear regression, there are two conventional approaches to evaluating goodness of fit: (1) examine residual model-data misfit systematically for non-random patterns which might indicate model deficiencies or incorrect weights for data and model, and (2) cross-validation using independent data (e.g., withholding data for comparison with the assimilation product). Problems identified during the validation process are critical to the improvement of the estimation. Ocean state estimation techniques will not advance without elaborate effort in evaluating the assimilation product.

Dynamical consistency

Some assimilation methods require correction of model state at the time instants when observations are available (e.g., sequential estimation methods). The correction, being an abrupt "jump" of estimate state, renders the estimate dynamically inconsistent. If it is not inverted back to specific processes (e.g., advection, diffusion, surface forcing, etc.), it would pose a difficulty in diagnosing physical processes such as analysis of tendencies in heat budget because of non-closure of budget. Estimation methods includes observations in the time dimension to correct the entire model trajectory, such as the adjoint method and Kalman filter/smoother, are advantageous in this regard but at the expense of the more complicated implementation and higher computational cost.

Multi-disciplinary collaborations

One factor hampering progress in ocean modeling and ocean state estimation is a weak link among modelers, data assimilators, and observationalists. Building computational machinery for assimilation is the primary responsibility of such groups like ECCO. However, evaluation and improvement of the assimilation product, and the underlying dynamical model, is a challenging task that should involve assimilators, modelers and observers. The tasks include:

- determining data and model errors and error statistics;
- preparing and quality controlling observations;
- pre-processing data for volume reduction (assimilation does not use satellite data at every pixel or current meter records at hourly intervals, but data reduction should not loose useful information);
- comparing model output with data and simple models to detect biases that may signal model deficiencies.

Given the diversity of observations and the complexity of state-of-the-art dynamical models to be applied for CLIVAR, active inputs from observationalists and from modelers are indispensable to a successful ocean state estimation effort.

The use assimilation products by scientists from areas other than physical oceanography is an important aspect. This is because observations of chemical, biological, and geological variables are not yet included by many major ocean data assimilation projects. The feedback from scientists other than physical oceanographers would help improve the quality of assimilation products.

Computational efficiency versus complexity of estimation methods

Ideally, state estimation should be done with the eddy-resolving models that have as complete physics as possible. Given today's computational resources, this is impractical for many advanced assimilation methods (e.g., adjoint, extended Kalman filter), which are computationally intensive. Therefore, compromises have to be made between the level of complexity in assimilation schemes and the level complexity in models (in terms of physics or resolution). While some prefers to use simpler assimilation method with complex and high-resolution modes, others use more advanced assimilation methods with simpler or lower-resolution models. Comparison of results obtained from these two types of efforts for the same problem would help identify the most effective way to proceed. Nevertheless, few groups have adequate resources to undertake such a task. Moreover, the relative merit of these two approach may be problem-dependent, which makes it difficult to generalize the finding to other applications.

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